26163-08-6 | DTXSID10737557

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.56

Global applicability domain: Inside

Local applicability domain index: 5.80e-01

Confidence level: 6.44e-01

Nearest Neighbors from the Training Set

Image not found
Cyclopropane
Measured: 1.72
Predicted: 1.56

Image not found
2-Butyne
Measured: 1.46
Predicted: 1.43

Image not found
2,5-Dihydrofuran
Measured: 0.46
Predicted: 5.82e-01

Image not found
Tetrahydrofuran
Measured: 0.46
Predicted: 6.00e-01